

Methanol

67-56-1 | DTXSID2021731

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -93.5 °C

Global applicability domain: Inside

Local applicability domain index: 4.91e-01

Confidence level: 4.80e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methanol</div> <div>Measured: -97.6</div> <div>Predicted: -93.5</div>	<div>Image not found</div> <div>Ethyl hydroperoxide</div> <div>Measured: -100</div> <div>Predicted: -75.6</div>	<div>Image not found</div> <div>Ethanol</div> <div>Measured: -114</div> <div>Predicted: -107</div>
<div>Image not found</div> <div>tert-Butyl hydroperoxide</div> <div>Measured: -8.00</div> <div>Predicted: -23.0</div>	<div>Image not found</div> <div>2-Methoxyethanol</div> <div>Measured: -85.1</div> <div>Predicted: -57.2</div>	